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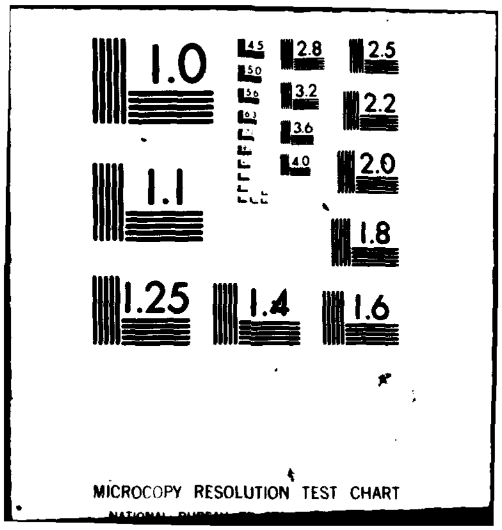
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)
The ~~Georgia Tech~~ program of research on ionic transport in gases is described. Experimental measurements of ionic mobilities and diffusion coefficients are discussed. The use of the mobility data to obtain ion-neutral interaction potentials is described. References to recent publications are given, and the program for the next year is outlined.

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The Drift, Diffusion, and Reactions of Slow Ions in Gases

O. N. R. SUMMARY QUESTIONNAIRE

Contract No. N00014-80-C-0243

Nov. 1, 1980 - Oct. 31, 1981

(1c) E. W. McDaniel [redacted] I. R. Gatland, Co-Principal Investigators
School of Physics, Georgia Institute of Technology
Atlanta, Georgia 30332

9 Rept. for 1 Nov 80-31 Oct 81

1. Contract Description

The current experimental program consists mainly of measurements of the mobilities and longitudinal diffusion coefficients of ions in various gases at room temperature. By varying the energy parameter (E/N) of the ions, we may vary the average ionic energy from the thermal value at 300°K to about 10 eV. The data are of immediate practical value in applications involving ionized gases. They are also used to test theoretical ion-neutral interaction potentials, to determine directly such interaction potentials, and to test theories of ionic transport in gases.

12

During the coming year, we propose to make accurate measurements of the mobilities and longitudinal diffusion coefficients of Na^+, Rb^+, and Cs^+ ions in molecular gases and of $T\ell^+$ ions in He, H_2, N_2, O_2, and CO_2 over a wide range of E/N, and to continue the program of obtaining interaction potentials.

The theoretical effort will involve a continuation and extension of the following studies now under way:

(1.) The determination of ion-neutral interaction potentials for various ion-gas combinations. Among the systems to be studied are $T\ell^+$ and $C\ell^-$ ions in inert gases.

(2.) Study of the phenomenon of ion runaway, and especially the transition from normal drift to runaway. Monte Carlo techniques are being used in an attempt to establish criteria for the onset of runaway in terms of the electric field intensity (E), the gas number density (N), and interaction parameters.

2. Scientific Problem

Our measurements of transport properties of ions in gases provide data of immediate practical use in the quantitative analysis of electrical discharges in the laboratory and in the explanation of various natural phenomena. However, the most important use of the drift velocity data will be to obtain information on ion-neutral interaction potentials, covering a very wide range

of ion-neutral separation distance, by inverting the experimental data. The interaction potential for a two-particle system is one of the most fundamental properties of the system. It determines the mutual scattering behavior of the particles and hence the transport properties. The interaction potential also determines many properties of the system that is formed if the two particles can temporarily or permanently combine. In the case of radiative processes, for example, the interaction potentials for the upper and ground states of a neutral diatomic molecule or ion are required for the determination of the wave functions, transition probabilities and spectral features. The standard beam scattering technique used to obtain information about the interaction potential for an ion-neutral system covers a much smaller range of separation distance than does the new method described here.

In addition, the experimental transport data may be used in the calculation of ion-ion recombination coefficients (see, for example, M. R. Flannery, "Ionic Recombination", in Atomic Processes and Applications (P. G. Burke and B. L. Moiseiwitsch, Eds.) North-Holland, Amsterdam (1976) pp. 407-466.)

We shall also calculate from our measured drift velocities the zero-field mobilities of these ions in various gases at temperatures ranging from 300^{o}K to $\sim 10^4$ ^{o}K by the techniques we have described. [See E. A. Mason, L. A. Viehland, H. W. Ellis, D. R. James, and E. W. McDaniel, "The Mobilities of K^+ Ions in Hot Gases", Phys. Fluids 18, 1070 (1975)]. Finally, we shall use our diffusion coefficients to test the theories of diffusion of gaseous ions in electric fields which have been developed during the last few years. [See L. A. Viehland and E. A. Mason, Annals of Physics 91, 499 (1975); 110, 287 (1978). S. L. Lin, L. A. Viehland and E. A. Mason, "Three-Temperature Theory of Gaseous Ion Transport", Chem. Phys. 37, 411 (1979). M. Waldman and E. A. Mason, Chem. Phys. 58, 121 (1981).]

3. Scientific and Technical Approach

The experiments are performed with a drift tube mass spectrometer,* by techniques which permit accurate measurements to be made on individual ionic

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*This instrument (abbreviated here as DTMS) is designed to operate at low pressures (usually well below 1 Torr). We also have a high pressure DTMS, which we occasionally use on the ONR research, although it is utilized mainly on research supported by NSF (see Section 10).

species even though several species may be simultaneously present and coupled by ion-molecule reactions. The drift tube gas is maintained at room temperature, but the average energy of a given species of ion can be varied from very close to thermal energy up to a maximum of about 10 eV in favorable cases. The average energy of the ions of a given type is determined by the parameter E/N, and measurements are made as a function of E/N.

The basic measurement made is of the arrival time spectra for each separate ionic species in the drift tube. The measurements are made as functions of drift distance, electric field strength in the drift region, number density of gas molecules in the drift tube, and the energy parameter. The theoretical calculations are concerned with the relation between the ion-neutral interaction potential and the measured values of the mobilities and diffusion coefficients. The calculation of the mobilities is based on a moment solution of the appropriate Boltzmann equation with basis functions which reflect the sometimes high random energy derived from the electric field and the non-symmetric character of the ionic velocity. This allows the mobility data to be used to test theoretical potentials and also to serve as an integral part of an iteration technique which determines the interaction potential directly from the data.

4. Progress

During the current O. N. R. contract period, we have measured, or expect to measure, the mobilities and longitudinal diffusion coefficients of Br^- in Kr and Ne and of $T\ell^+$ in Xe, Kr, Ar, and possibly Ne. These measurements were (or will be) performed at 300^oK and over the widest possible range of E/N. Our study of Li^+ - Xe has also been completed.

The theoretical studies have concentrated on two points: one being the understanding of runaway and the other being the determination of interaction potentials from the drift data. As regards runaway, a variable cutoff Coulomb potential has been adopted and its momentum transfer cross section is being compared with that for H^+ - He scattering. Also a Monte Carlo simulation with this model potential is being used to investigate the ion velocity distribution.

Interaction potentials have been developed for three systems; Br^- - Ar, Br^- - Kr, and Br^- - Xe. The case of $T\ell^+$ - Xe will be studied next and may be followed by $T\ell^+$ - Kr.

5. Publications (Asterisk denotes O. N. R. Research)

* Mobility of Cl^- Ions in Xe, and the Cl^- - Xe Interaction Potential," M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, E. W. McDaniel and I. R. Gatland, J. Chem. Phys. 73, 3183 (1980).

"Compilation of Atomic and Molecular Data Relevant to Gas Lasers," E. W. McDaniel, Redstone Arsenal, Alabama; U. S. Army MICOM Technical Report H-78-1. Vols. VII and VIII, (Dec. 1980).

"Temperature Dependent Mobilities: NO_2^-, NO_3^-, CO_3^-, CO_4^-, and O_2^+ in O_2," M. D. Perkins, F. L. Eisele and E. W. McDaniel, J. Chem. Phys. 74, 4206 (1981).

* "Mobilities and Interaction Potentials for K^+ - Ar, K^+ - Kr, and K^+ - Xe," D. R. Lamm, M. G. Thackston, F. L. Eisele, H. W. Ellis, J. R. Twist, W. M. Pope, I. R. Gatland and E. W. McDaniel, J. Chem. Phys. 74, 3042 (1981).

"Measurement of the Mobilities of Cl^-, $NO_2^-.H_2O$, $NO_3^-.H_2O$, $CO_3^-.H_2O$, and $CO_4^-.H_2O$ as a Function of Temperature," F. L. Eisele, M. D. Perkins, and E. W. McDaniel, J. Chem. Phys. 75, 2473 (1981).

* "Longitudinal Diffusion Coefficients and Test of the Generalized Einstein Relation for Br^- - Ne, Br^- - Ar, Br^- - Kr, and Br^- - Xe," F. B. Holleman, W. M. Pope, F. L. Eisele, J. R. Twist, G. W. Neeley, M. G. Thackston, R. D. Chelf, and E. W. McDaniel, submitted to J. Chem. Phys. (in press).

* "The Determination of Potentials for Ion-Atom Interactions by Ion Mobility Experiments", by I. R. Gatland, Invited Paper, Second International Swarm Seminar, Oak Ridge, Tenn., July 22-23 (1981).

* "The Mobilities and Interaction Potentials of Br^- - Ne, Br^- - Ar, Br^- - Kr, and Br^- -Xe," D. R. Lamm, I. R. Gatland, F. L. Eisele, J. R. Twist, M. G. Thackston, R. D. Chelf, F. B. Holleman, and E. W. McDaniel, submitted to J. Chem. Phys.

The Transport Properties of Ions in Gases, by E. A. Mason and E. W. McDaniel, Wiley, New York, in preparation.

Applied Atomic Collision Physics (Ed. by H. S. W. Massey, E. W. McDaniel, and B. Bederson), 5 vols., Academic, New York, in press.

"Transport Properties of Gaseous Ions- Part III", H. W. Ellis, E. A. Mason, and E. W. McDaniel, to be submitted to Atomic Data and Nuclear Data Tables.

* "The Mobilities and Longitudinal Diffusion Coefficients of Li^+ Ions in Kr and Xe", J. R. Twist, M. G. Thackston, G. W. Neeley, F. B. Holleman, R. D. Chelf, and E. W. McDaniel, submitted to J. Chem. Phys.

* "Rate-Sensing Servo Amplifier for Increasing the Stability of Servo-Controlled Leak Valves," J. R. Twist, Rev. Sci. Instr., in press.

* "Ion Mobility Tests of Li^+ - Ar Potentials", I. R. Gatland, J. Chem. Phys. 75. 4162 (1981).

6. Extenuating Circumstances

Our low-pressure DTMS has been in operation since 1967, with an average of only approximately 5% downtime due to equipment failure until about March 1, 1980. At about this time we began to encounter a series of electrical and mechanical problems which cost us months of running time. The Granville Phillips Servo Leak Controller developed intermittent instabilities, and satisfactory operation was restored only by overhauling the unit, and designing, testing, and constructing a Signal Conditioning Circuit. A commercial Freon Cooler was installed in the gas feed line to save liquid nitrogen costs; this device broke down and had to be returned to the manufacturer, temporary measures being adopted until its repair and return. A power outage during a storm on a weekend, combined with an equipment failure in our laboratory, resulted in the loss of a forepump, but the diffusion pumps were reactivated when the power was restored. This accident caused the apparatus to be exposed to hot pump oil vapor and necessitated a cleanup, gold-plating, and reassembly that consumed several months.

However, we were able to take some advantage of the downtime and disassembly of the DTMS. The interior surfaces are now cleaner than at any time since the early days of operation. Several valves, manifolds, pressure gauges, and fittings have been replaced. Automatic quick cools have been installed on the diffusion pumps, and a new safety circuit for control of the electrical power is on line. We appear to be fully protected against power and forepump failure, and the DTMS is in much improved overall condition.

7. Unspent Funds Remaining at End of Current Contract Period

None.

8. Personnel Involved in the Research

(A) E. W. McDaniel, Regents' Professor of Physics - Project Director.

(B) I. R. Gatland, Professor of Physics - Co-Principal Investigator.

(C) J. R. Twist, Postdoctoral Fellow. Dr. Twist obtained his Ph.D. degree in Atomic Physics from the University of Oklahoma in June, 1979 and began work with us at that time on a two-year appointment.

(D) M. G. Thackston, Graduate Student and Postdoctoral Fellow. Mr. Thackston joined us in the summer of 1975 and did his Ph.D. research with us. He is continuing his work as a Post-Doctoral Fellow.

(E) Mark Byers - Graduate Research Assistant. Mr. Byers entered graduate school in Physics here in September, 1981 and joined our research group at that time.

(F) D. R. Lamm, Graduate Student. Mr. Lamm began work with us in October, 1979 on the theoretical aspects of our program for his Ph.D. research.

(G) F. B. Holleman, Graduate Research Assistant. Mr. Holleman joined our group in June, 1980, when he entered graduate school at Georgia Tech.

(H) R. D. Chelf, Graduate Research Assistant. Mr. Chelf started to work with us in October, 1980, when he passed the Comprehensive Examinations in Physics. He is now doing his P.D. thesis research with us.

(I) Conrad Norman, High-School Student. Mr. Norman worked with us as a minority research apprentice during the summer of 1981.

9. Graduate Students Who Earned Advanced Degrees During Contract Period

Mr. Thackston received his Ph.D. degree in Physics in March, 1981.

10. Other Government-Sponsored Research

We have recently obtained from the National Science Foundation a two-year extension of their support, the extension providing $136,699 for a program entitled "Measurement of Ion Transport Properties, Ion Reaction Rates, and Trace Neutral Concentrations of Atmospheric Interest". The Grant Number is ATM-8016881. The NSF Grant is scheduled to end on August 31, 1982. The NSF research involves measurements of ionic mobilities and reaction rates that are of atmospheric interest. Practically all of the measurements will be made with our high-pressure DTMS. There is no overlap between the research proposed to ONR in this document and that performed with NSF support, although equipment and personnel (E. W. McDaniel) will be shared.

We have no proposals outstanding at this time.